The two-body problem of ultra-cold atoms in a harmonic trap

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Abstract

We consider two bosonic atoms interacting with a short-range potential and trapped in a spherically symmetric harmonic oscillator. The problem is exactly solvable and is relevant for the study of ultra-cold atoms. We show that the energy spectrum is universal, irrespective of the shape of the interaction potential, provided its range is much smaller than the oscillator length.

I. INTRODUCTION

From the earliest studies of the dynamics of our solar system to the first attempts to apply quantum mechanics to the simplest atoms (hydrogen and helium), few-body systems have played a pivotal role. In particular, the problem of two particles interacting via a central force law is familiar to students of physics. After elimination of the center-of-mass motion the two-body problem is reduced to a one-body problem in the relative co-ordinate. The well-known two-body gravitational and the Coulomb problems admit exact analytical solutions, which can be tested by experiments.

The few-body problem is still of great interest, especially in view of recent experimental advancements in the area of ultra-cold atoms.[1,2] In these experiments neutral atoms are first cooled to nano-Kelvin temperatures and then confined in an optical lattice formed by standing wave laser beams, where there are as few as two-and three atoms per lattice site. Typically, the lattice sites confining the atoms may be regarded as harmonic oscillator potentials with a trapping frequency ν of a few tens of cycles per second. The coupling between the harmonic oscillator wells (that is, between the lattice sites) may be controlled by the intensity of the laser beams. In the limit of low tunneling, the individual wells may be regarded as independent three-dimensional (3D) harmonic oscillators. The strength of the pair-wise interaction between the atoms on each site may be fine-tuned by sweeping through a static magnetic field using a Feshbach resonance.[3,4,5] At nano-Kelvin temperatures quantum effects dominate, and we thus have what amounts to a non-relativistic quantum few-body system whose inter-particle interactions can be controlled at will. This achievement is truly remarkable, and such ultra-cold matter experiments can serve as ideal laboratories to investigate the quantum few-body problem.

The experimental group of Stöferle *et al.*[2] has trapped two ^{40}K atoms in a 3D harmonic oscillator well, and by tuning near the Feshbach resonance, can make the inter-particle interaction strong enough to form diatomic molecules. Because the two atoms (each of which behaves as a fermion[6]) occupy distinct hyperfine states, they may still interact in the relative s-state. Subsequently, the energy of the state is deduced by dissociating the molecule using an rf-pulse and measuring the binding energy of the molecule. The binding energy as a function of the strength of the interaction (which is related to the s-wave scattering length) is mapped out by by sweeping a magnetic field using a Feshbach resonance. In these

experiments the atoms form only loosely bound pairs so that the interaction range may be taken to be very small compared to the size of the two-body system. This system is then an experimental realization of the exactly solvable problem of two harmonically trapped particles interacting via a zero-range pair-wise potential at zero temperature.

In this article we present the exact solution to this quantum two-body problem, assuming only a knowledge of quantum mechanics at the senior undergraduate or beginning graduate student level. Remarkably, this ostensibly simple problem has only been investigated within the last 10 years,[7,8,9] and now enjoys a new life due to its relevance to the experiments discussed in Ref. 2. In particular, the theoretical spectrum of this system is in excellent agreement with the experimental spectrum we have described.[7] Our approach does not make any reference to the shape of the short-range two-body potential, and requires only that its range be much smaller than the oscillator length,[7] which serves as a natural measure of the particle spacing. This approach beautifully illustrates the notion of shape-independence of potentials (for low energy scattering and binding) that was first developed in the context of nuclear physics.[10] Shape-independence is embodied in the effective range expansion, which is explained and derived in Ref. 11. The concepts of scattering length and effective range that come in this expansion are important in the analysis of the experimental results with ultra-cold atoms, and readers are encouraged to study the excellent discussion of these topics in Ref. 10. We shall make use of these concepts and show that the energy levels of this system are independent of the shape of the interaction potential in the limit of zero range. This result is accomplished by noting that, for a harmonic trap, the center of mass motion may be isolated, and the interacting relative motion may be written as a one-body problem. The irregular solution of the harmonic oscillator wave function, which is normally discarded in the noninteracting problem, will be shown to be the relevant solution for the zero-range interacting case. This realization paves the way for a gentle introduction to the concept of a pseudopotential in the form of a regularized delta function.

The zero-range pseudopotential, first introduced by Fermi,[12] and applied to the many-body problem by Huang and Yang,[13] is extensively used in the current literature of ultra-cold gases.[14] The same pseudopotential has also been used to study the spectrum of two particles interacting by a zero-range potential in a spherical harmonic oscillator well.[7] Rather than taking this path, we shall follow the derivation of Jonsell,[8] which is in the same spirit as our initial intuitive approach. In Sec. III we finish with some concluding remarks and suggestions

for future research in this area.

II. THE TWO-BODY PROBLEM

A. The zero-range pseudopotential

We first consider the problem of two identical bosons, each of mass M, in the absence of a confining potential. The bosons interact with a short-range central potential. Most of what follows in this section also applies to fermionic atoms in the spin-singlet state, or to nucleons in the s-state with an antisymmetric spin-isospin wave function.[15] In the relative co-ordinate $r = |\mathbf{r_1} - \mathbf{r_2}|$ the s-state asymptotic scattering wave function for positive energy E is given by

$$u(r) = r\psi(r) \sim \sin(kr + \delta(k)), \quad (r > b). \tag{1}$$

We have $E = \hbar^2 k^2/M$, and b is the range of the potential. The effective range expansion, relating the phase shift to the scattering length a and the effective range r_0 is given by[16]

$$k \cot \delta(k) = -\frac{1}{a} + \frac{1}{2} r_0 k^2 - P r_0^3 k^4 + Q r_0^5 k^6 + \ldots \tag{2}$$

Potentials of different shapes may have identical values of a and r_0, but the parameters P and Q are shape-dependent. Figure 1 schematically illustrates the zero-energy wave function $u(r)$ for an attractive square-well potential,

$$V(r) = -V_0 \Theta(b - r), \tag{3}$$

of depth V_0 and range b; $\Theta(x)$ is the usual unit Heaviside function.

Figure 1 depicts a situation where the intercept of the the zero-energy wave function (or its extrapolation) on the horizontal axis is the scattering length a, with its sign signifying the presence or absence of a bound state. For a shallow potential that supports no bound state, the scattering length a is negative (Fig. 1(a)). When the depth of the potential is increased and fine-tuned as in Fig. 1(b), the system has a zero-energy "bound" state corresponding to $a \to \pm\infty$. For this limiting case the dimensionless quantity $\gamma = MV_0 b^2/\hbar^2$ equals $\pi^2/4$. The corresponding values of γ for other two-parameter attractive potentials are listed in Ref. 17. A further increase in the depth results in supporting only one bound state, and the scattering length a is shown to be positive (Fig. 1(c)).

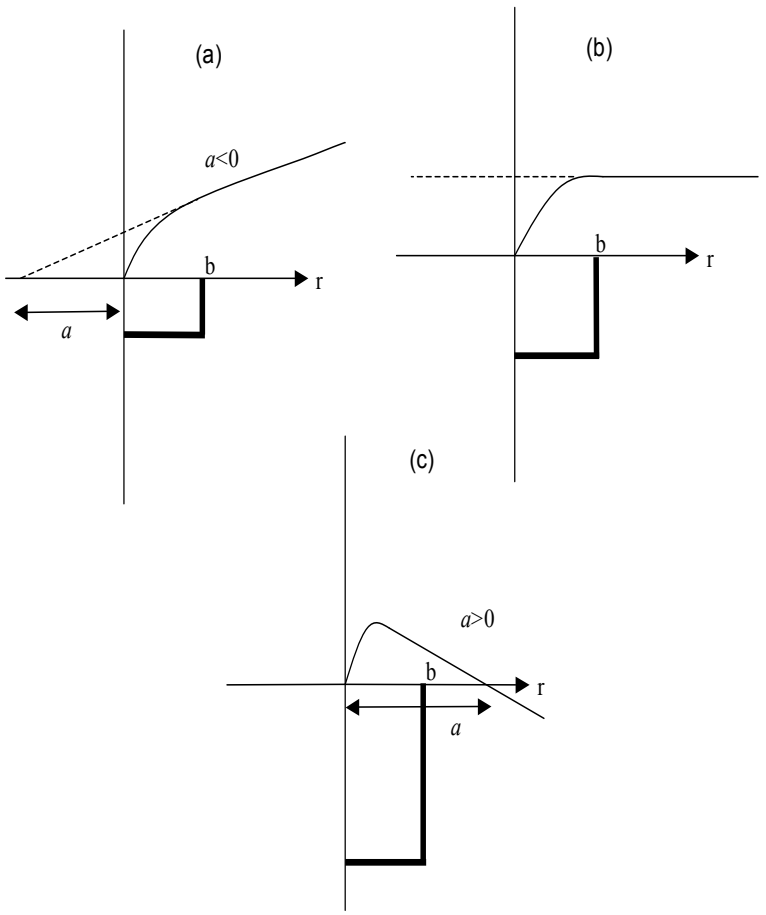

FIG. 1: An attractive spherical square well potential. The thin solid line indicates the zero-energy wave function $u(r)$, and the dashed line the extrapolated asymptote. (a) Shallow well with negative scattering length. (b) Depth tuned to $V_0 = \pi^2\hbar^2/4Mb^2$ with $a \to \infty$ corresponding to the zero energy bound sate. (c) A deeper well supporting only one bound state and positive scattering length. Note that $u(r) \sim (r - a)$ for $r > b$.

The situation is more complicated when the depth of the potential becomes still stronger to support two or more bound states. For the case of the square-well example, it may be shown that the s-wave scattering length is given by[15]

$$a = b\left(1 - \frac{\tan\sqrt{\gamma}}{\sqrt{\gamma}}\right). \tag{4}$$

Therefore $\sqrt{\gamma} = 3\pi/2$ signals the appearance of the next zero-energy bound state, with the scattering length changing sign. A further increase results in two bound states. Note from Eq. (4) that the scattering length a depends on the range b of the potential and its strength γ. In what follows we shall be interested in taking the zero-range limit of the interaction,

while keeping the strength parameter γ fixed.

The effective range r_0 is proportional to the range b of the potential, and goes to zero as $b \to 0$. For this case Eq. (2) reduces to

$$k \cot \delta = -\frac{1}{a}. \tag{5}$$

For positive a we may extrapolate Eq. (5) to a bound state. Note that the S-matrix for the s-state is defined as $S(k) = \exp(2i\delta(k))$, and the S-matrix has a simple pole for each bound state in the upper half of the imaginary k-axis on the complex k-plane.[18] A zero-range potential can support only one bound state. At a bound state therefore, $k = i\kappa$, and $\cot \delta = i$. The relation (5) for a zero-range potential then reduces to $\kappa = 1/a$. Hence the binding energy $B = -E$, and the bound state wave function $\psi(r)$ is given by

$$\psi(r) = \frac{\exp(-r/a)}{r}, \quad (r > 0), \tag{6}$$

$$B = \hbar^2/Ma^2. \tag{7}$$

Equation (6) is exact for a zero-range potential. If r_0 is nonzero, the relations for B and the asymptotic ($r > b$) wave function ψ are approximately true only if the binding B is close to zero, which implies that $a \gg r_0$, and the system is large in size compared to the range of the potential. As an example where these conditions are only marginally satisfied, consider the deuteron, which is the lightest stable atomic nucleus, and is a bound state of a neutron and a proton. The n-p scattering length in the s-state ($S = 1$, $T = 0$) is $a = 5.43\,\mathrm{fm}$, and $r_0 = 1.75\,\mathrm{fm}$, where $1\,\mathrm{fm} = 10^{-15}\,\mathrm{m}$. Equation (7) for the binding energy gives $B = 1.41\,\mathrm{Mev}$, compared with the experimental value of 2.23 Mev.[19]

Because r_0 is nonzero but is much smaller than a, this agreement could be improved by taking the next term in the expansion in Eq. (2). Following the same extrapolation for the bound state at $k = i\kappa$, we obtain the quadratic equation

$$\kappa = \frac{1}{a} + \frac{1}{2} r_0 \kappa^2. \tag{8}$$

We select only the root that gives $\kappa = 0$ when $a \to \infty$ and $r_0 = 0$ and obtain

$$\kappa = \frac{1}{r_0}\left(1 - \sqrt{(1 - 2r_0/a)}\right). \tag{9}$$

Equation (9) for the deuteron gives $B = 2.16\,\mathrm{MeV}$, which is close to the experimental value.[20]

We have assumed that the size of the bound two-body system is much larger than the range of the potential responsible for the binding. The details of the potential at short distances do not manifest themselves significantly in the wave function, and the binding is determined by the low energy scattering parameters. It should therefore be possible to design an effective potential that reproduces the shape-independent results we have obtained. Such an effective one-parameter pseudopotential is easily derived using the wave function $\psi(r)$ given by Eq. (6). From the relation $\nabla^2(1/r) = -4\pi\delta^3(r)$ we obtain $-\nabla^2(\exp(-r/a)/r) = -a^{-2}\exp(-r/a)/r + 4\pi\exp(-r/a)\delta^3(r)$. If we identify $\exp(-r/a)/r = \psi(r)$, we may write

$$-\nabla^2\psi + 4\pi a\delta^3(r)\frac{\partial}{\partial r}r\psi = -\frac{1}{a^2}\psi. \tag{10}$$

We see that the pseudopotential

$$V(r) = \frac{\hbar^2}{M}4\pi a\delta^3(r)\frac{\partial}{\partial r}r \tag{11}$$

reproduces the earlier results for the wave function and the binding energy of any zero-range potential with a given scattering length. In the many-body problem of an ultra-cold dilute gas, where $k \to 0$, and the average distance between the particles is much larger than the range b of the potential, the same regularized pseudopotential in Eq. (11) is widely used.[13,14] Note that $\partial(r\psi)/\partial r$ in the limit $r \to 0$ is $\psi(0)$ for a wave function that is well-behaved at the origin. In addition, it also gives a finite result for the irregular $\psi(r)$ that goes as r^{-1}, which is more relevant for our problem.

B. Two particles in a harmonic potential

First consider the case of noninteracting particles. Each particle of mass M moves in a harmonic potential $1/2M\omega^2r^2$. If we make the usual transformations to center-of-mass and relative co-ordinates, $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)$, and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and their corresponding canonical momenta $\mathbf{p}$ and $\mathbf{P}$, we obtain

$$H_0 = (\frac{P^2}{2M_{\rm cm}} + \frac{1}{2}M_{\rm cm}\omega^2R^2) + (\frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2r^2), \tag{12}$$

where $M_{\rm cm} = 2M$ and $\mu = M/2$. We concentrate on the relative motion and divide the relative distance r by $\sqrt{\hbar/\mu\omega}$ and the energy E by $\hbar\omega$. In terms of the dimensionless scaled variables $x = r/\sqrt{2}l$, where $l = \sqrt{\hbar/(M\omega)}$, and $\eta = 2E/(\hbar\omega)$, the Schrödinger equation for

the relative wave function $u(r) = r\psi(r)$ in the s-state is given by

$$-\frac{d^2u}{dx^2} + x^2u = \eta u. \tag{13}$$

The regular ground state solution is $u_0(x) = x\exp(-x^2/2)$, corresponding to $\psi(x) = \exp(-x^2/2)$, with $\eta = 3$, or $E = \frac{3}{2}\hbar\omega$. It is easily checked that Eq. (13) is also satisfied for $x > 0$ by $u(x) = \exp(-x^2/2)$, corresponding to $\psi(x) = \exp(-x^2/2)/x$ with $\eta = 1$ or $E = \frac{1}{2}\hbar\omega$. Although normalizable and lower in energy, it is excluded as a valid solution in the noninteracting problem because at $r = 0$, the kinetic operator ∇^2 acting on $1/r$ would yield a delta function.

The situation changes for the zero-range interaction that we have been considering. At $r = 0^+$ we may ignore the harmonic confinement, and the wave function is given by Eq. (6). Even for nonzero b the harmonic potential may be ignored if $\mu\omega^2 b^2 \ll \hbar\omega$, which yields the condition $b/l \ll 1$ for the validity of the spectrum derived in the following. For the scattering length $a \to \infty$, the wave function is $1/r$, and smoothly joins with the irregular wave function above for $\eta = 1$ This analytic behavior suggests that the valid (normalized) ground state wave function in the limit of $a \to \infty$ for $r > 0$ is the irregular solution,

$$\psi(x) = \sqrt{\frac{2}{\pi^{3/2}}}\frac{\exp(-x^2/2)}{x}, \tag{14}$$

with $E = \frac{1}{2}\hbar\omega$. The next excited $\ell = 0$ state has one node, and by demanding that it be orthogonal to the the ground state given by Eq. (14), may be deduced to be $(x^2 - 1/2)\exp(-x^2/2)/x$, with energy $E = \frac{5}{2}\hbar\omega$. There is an infinite tower of such radially excited states with $\ell = 0$. This result is confirmed by our numerical calculations with the two-body potential

$$V(r) = -V_0\mathrm{sech}^2(r/b). \tag{15}$$

This potential has a bound state at $E = 0$ in free space when $V_0 = 8\hbar^2/Mr_0^2$, and $b = r_0/2$. With these parameters, the scattering length a is infinite, and the effective range is r_0. Figure 2 displays the first five eigenvalues as a function of r_0/l. Note that as $r_0 \to 0$, E in units of $\hbar\omega$ approaches $1/2, 5/2, 9/2, \ldots$.

The tower of states described above, for $a \to \infty$, may be generalized for any given a, following Ref. 8. From our previous considerations it is reasonable to assume that the general solution for $x > 0$ is of the form $u(x) = \exp(-x^2/2)f(x)$. It is convenient to let $y = x^2$, and

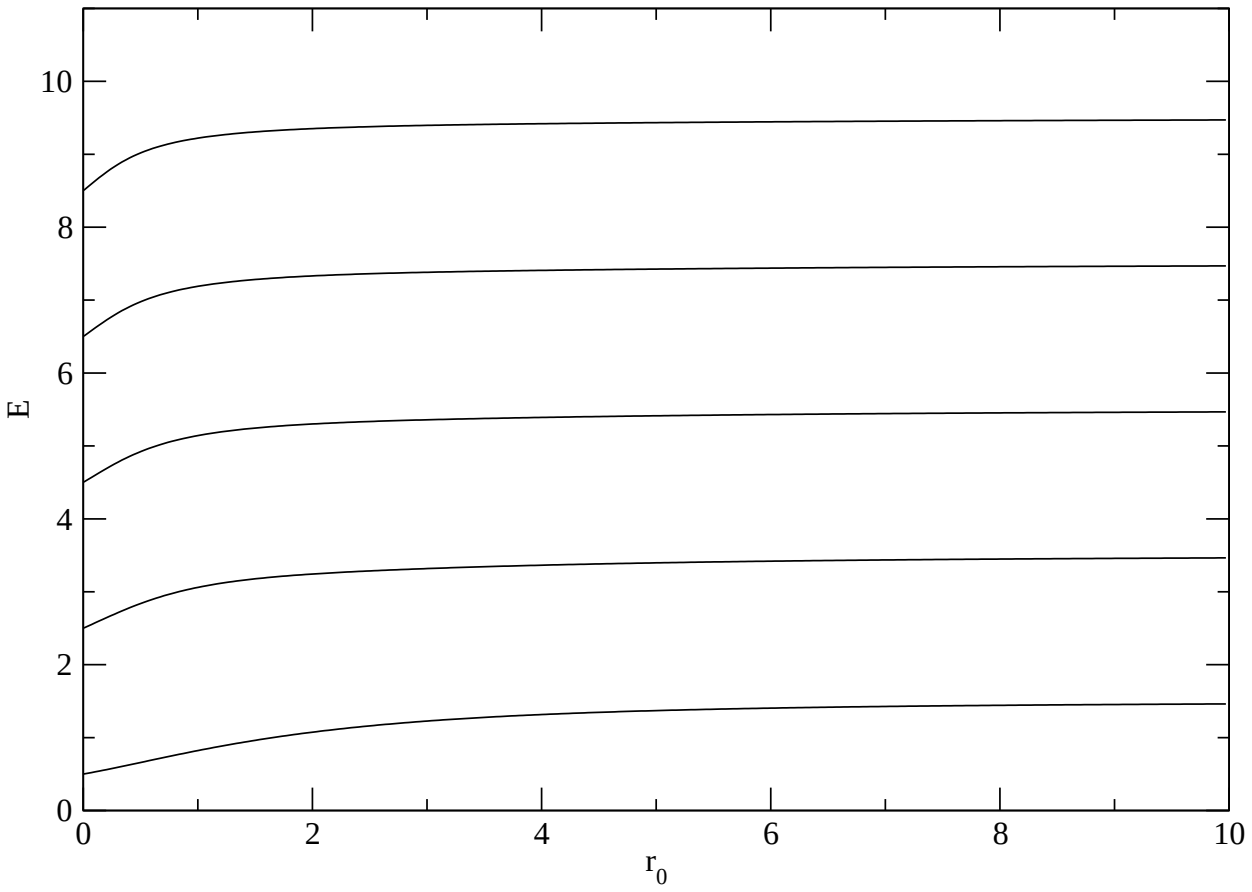

FIG. 2: The lowest five $\ell = 0$ energy levels for the potential $V(r) = -(8\hbar^2/Mr_0^2)\mathrm{sech}^2\left(\frac{2r}{r_0}\right)$, as r_0 is decreased toward zero. In this and all subsequent figures, lengths and energies are scaled as described in the text.

$w(y) = f(x)$. After some algebra, Eq. (13) is transformed to

$$y\frac{d^2w}{dy^2} + (\frac{1}{2} - y)\frac{dw}{dy} + (\frac{\eta - 1}{4})w = 0. \tag{16}$$

Equation (16) is the equation satisfied by the confluent hypergeometric function, and the solution is given by[21] $w(y) = c_1 M((1-\eta)/4, 1/2, y) + c_2 y^{1/2} M((3-\eta)/4, 3/2, y)$, where c_1 and c_2 are constants. We transform back to the x co-ordinate and obtain

$$u(x) = \left[c_1 M((1-\eta)/4, 1/2, x^2) + c_2 x M((3-\eta)/4, 3/2, x^2)\right] \exp(-x^2/2). \tag{17}$$

The ratio c_1/c_2 may be determined by noting that for large y, $M(p, q, y) \sim \Gamma(q)/\Gamma(p) y^{(p-q)} \exp(y)$. The large x behavior of the solution $u(x)$ given in Eq. (17) is

$$u(x) \sim \left[c_1 \frac{\Gamma(1/2)}{\Gamma((1-\eta)/4)} + c_2 \frac{\Gamma(3/2)}{\Gamma((3-\eta)/4)}\right] x^{-(1+\eta)/2} \exp(x^2/2). \tag{18}$$

For $u(x)$ not to diverge for large x, the quantity in the square brackets must vanish, yielding the ratio to be

$$\frac{c_1}{c_2} = -\frac{1}{2}\frac{\Gamma((1-\eta)/4)}{\Gamma((3-\eta)/4)}. \tag{19}$$

We now relate this ratio to the scattering length a to determine the eigenvalue η. We already noted that as $r \to 0^+$, the oscillator potential goes to zero, and $u(r)$ for positive energy is a scattering solution outside the zero-range potential, given by Eq. (1). For small r we have to within an overall constant,

$$u(r) \simeq (r + \frac{1}{k}\tan\delta). \tag{20}$$

In contrast, because the confluent hypergeometric functions go to unity for $x \to 0^+$, we find from Eq. (17), $u(x) \sim (c_1 + c_2 x)$. If we factor c_2 out of this expression and rewrite u in terms of the variable r, we find to within an overall constant,

$$u(r) \simeq \left(r + \sqrt{2}l\frac{c_1}{c_2}\right). \tag{21}$$

We compare Eqs. (20) and (21) and obtain

$$\frac{1}{k}\tan\delta = \sqrt{2}\ l\frac{c_1}{c_2}. \tag{22}$$

We substitute $\tan\delta = -ak$ in Eq. (22) and the ratio c_1/c_2 from Eq. (19) and obtain the desired relation

$$\frac{a}{l} = \frac{1}{\sqrt{2}}\frac{\Gamma((1-\eta)/4)}{\Gamma((3-\eta)/4)}. \tag{23}$$

The Gamma function diverges when its argument is zero or a negative integer. Hence, for $a \to \infty$, $\eta = 1, 5, 9, \ldots$, confirming our earlier results for both the energy spectrum and the corresponding wave functions $u(x)$.

Note that Eq. (23) has been obtained with no mention of the shape of the potential and is therefore applicable for any short-range two-body potential. This general analysis is in contrast with the derivation in Ref. 7 in which explicit use of the properties of the pseudopotential (11) was required.

Figure 3 displays the variation of the eigenvalues E (in units of $\hbar\omega$) as a function of a/l. For comparison we also give the values obtained numerically for a square-well potential with $b/l = 0.01$. On the scale of the plots, it is difficult to distinguish between the results. Note also that the ground state energy diverges toward $-\infty$ as $a \to 0$. This behavior is the same

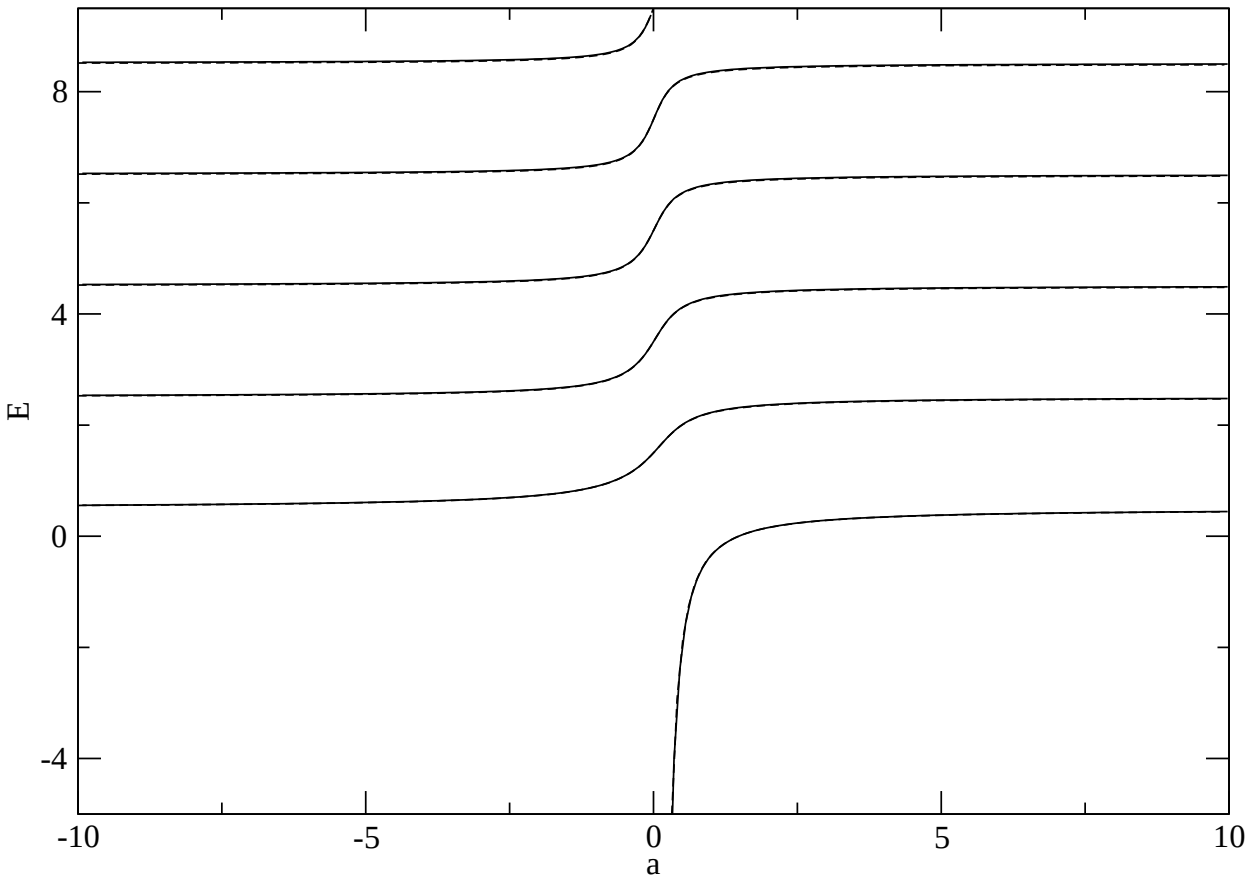

FIG. 3: The energy spectrum of the two-particle system in a harmonic trap. The solid lines are for the attractive square-well potential (3) with $b/l = 0.01$, and the dashed lines for the pseudopotential (11). This theoretical spectrum with varying scattering length is in excellent agreement with the experimentally measured binding energies of the dimers formed from ^{40}K atoms.[2]

as that of the a^{-2} divergence of the single bound state for the regularized delta function potential given by Eq. (6). Note that a zero scattering length does not necessarily mean that the interaction is zero. If the scattering length approaches 0 from the negative side (see Fig. 1(a)), the interaction becomes weaker and eventually vanishes. If it approaches zero from the positive side (see Fig. 1(c)), the interaction becomes stronger and stronger, squeezing the wave function more and more inside the potential. The flow of the eigenvalue curves as a function of a are to be understood with these observations in mind. Starting from the left in Fig. 3 with large negative a, the interaction becomes weaker a increases, eventually reaching zero when $a \to 0^-$. At this value we recover the unperturbed eigenvalues of the harmonic oscillator. To explain the behavior of the curves in Fig. 3 for $a > 0$, start

from the right-hand end and decrease a. We have already commented on the diverging ground state. The next one, starting at 5/2 at the right end, continually becomes less as a decreases, because the interaction becomes stronger, eventually reaching the lower value 3/2 at $a = 0^+$. The previous arguments should help to demystify the counterintuitive features of the pseudopotential discussed in Ref. 7.

III. CONCLUSIONS

We have discussed the two-body problem in the context of ultra-cold atoms. We have shown that the energy spectrum is a universal property of the interacting two-body problem provided that the range of the interaction is much smaller than the oscillator length. We have clarified the relation between the irregular solution and the regularized δ-pseudopotential. We invite the interested reader to apply the methods used here to the interesting one- and two-dimensional analogues of this problem. The energy spectra for these cases are also given in Ref. 7. The two-dimensional case is elaborated in Ref. 22. We suggest Ref. 23 and 24 for background reading on one- and two-dimensional scattering.

Acknowledgments

We would like to thank Yi Liang and Don Sprung for going through the manuscript carefully, and both of the anonymous referees for their very useful suggestions. This research was financed by grants from NSERC (Canada).

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[6] For a neutral atom the number of protons in the nucleus equals the number of electrons. So whether the atom as a whole behaves as a boson or fermion is determined by the neutron number being either even or odd. ^{40}K has 21 neutrons, and so as a whole behaves like a fermion.

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